LLNL-SR-414762

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# Progress Report on Collaborative Research on the Development of Chelators for a Surface Decontamination Foam

M. Sutton

July 15, 2009

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

# Lawrence Livermore National Laboratory

# Progress Report on Collaborative Research on the Development of Chelators for a Surface Decontamination Foam

## - June 30th, 2009 -

**Mark Sutton, PhD.**

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# Cs, Sr & Co – Chelate Models

**Running the models:**

Chemical thermodynamic modeling using data from the NIST Critical Stability Constant Database v46.

No data available for Cs DTPA and Cs NTA.

Not kinetic – assumes complete reaction.

1 micromolar metal solutions.

1 micromolar to 1 molar chelator solution.

Titrate pH.

Some models did not converge at high chelate concentration.

# Cs, Sr & Co – Chelate Models

**Data Caveats:**

Data show optimum pH and chelate concentration for maximum chelator efficiency.

Models do not show speciation….

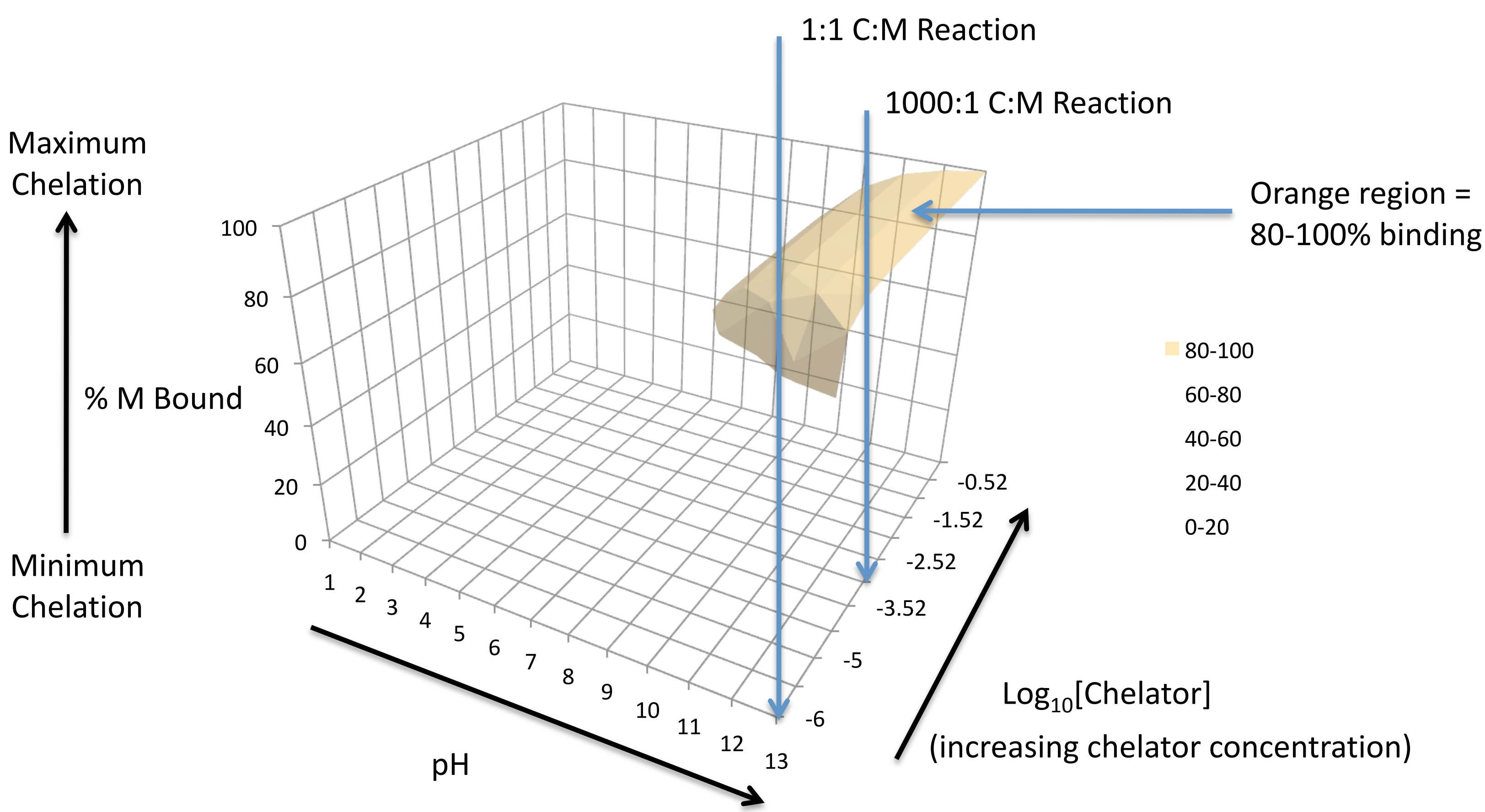
EDTA binds lots of metals effectively (i.e. non-specific).

EDTA shows >60% efficiency for Cs at high pH, but in the real world (with natural background levels of other metals), EDTA will never bind Cs efficiently.

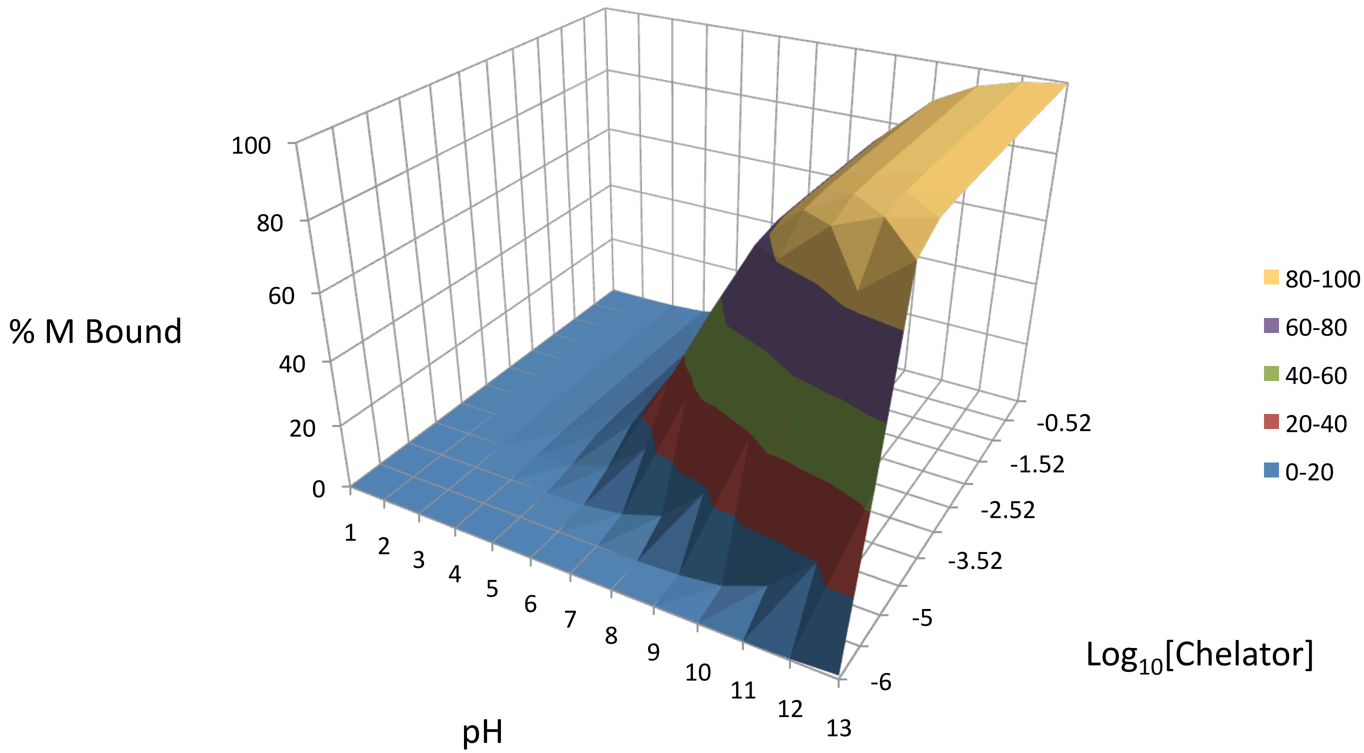
However, it is possible to vary pH to alter EDTA specificity for Co in a mixture of Sr and Cs….

EDTA binds to Co at pH 2-12, Sr at pH 4-12 and poorly to Cs. Therefore, to selectively bind Co, maintain pH <4.

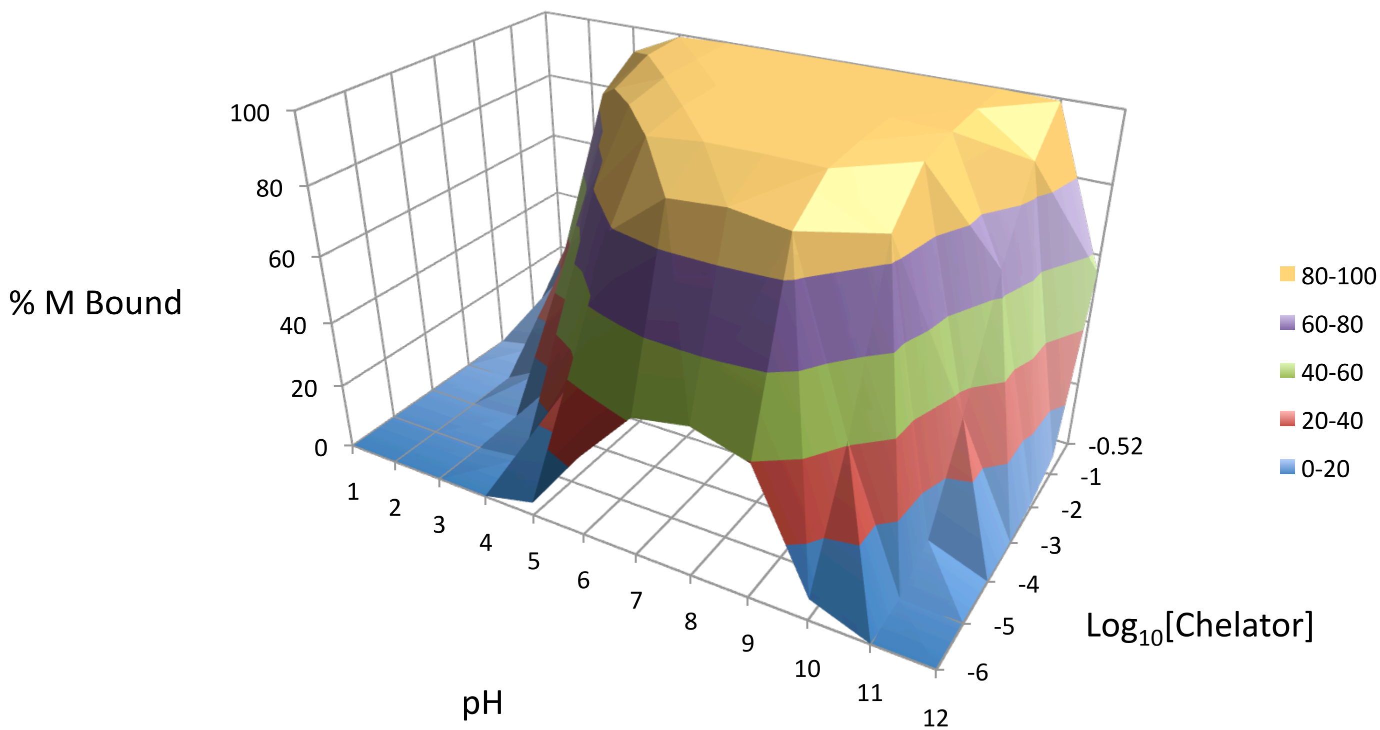
# M – Chelate Contours



# Cs – Prussian Blue

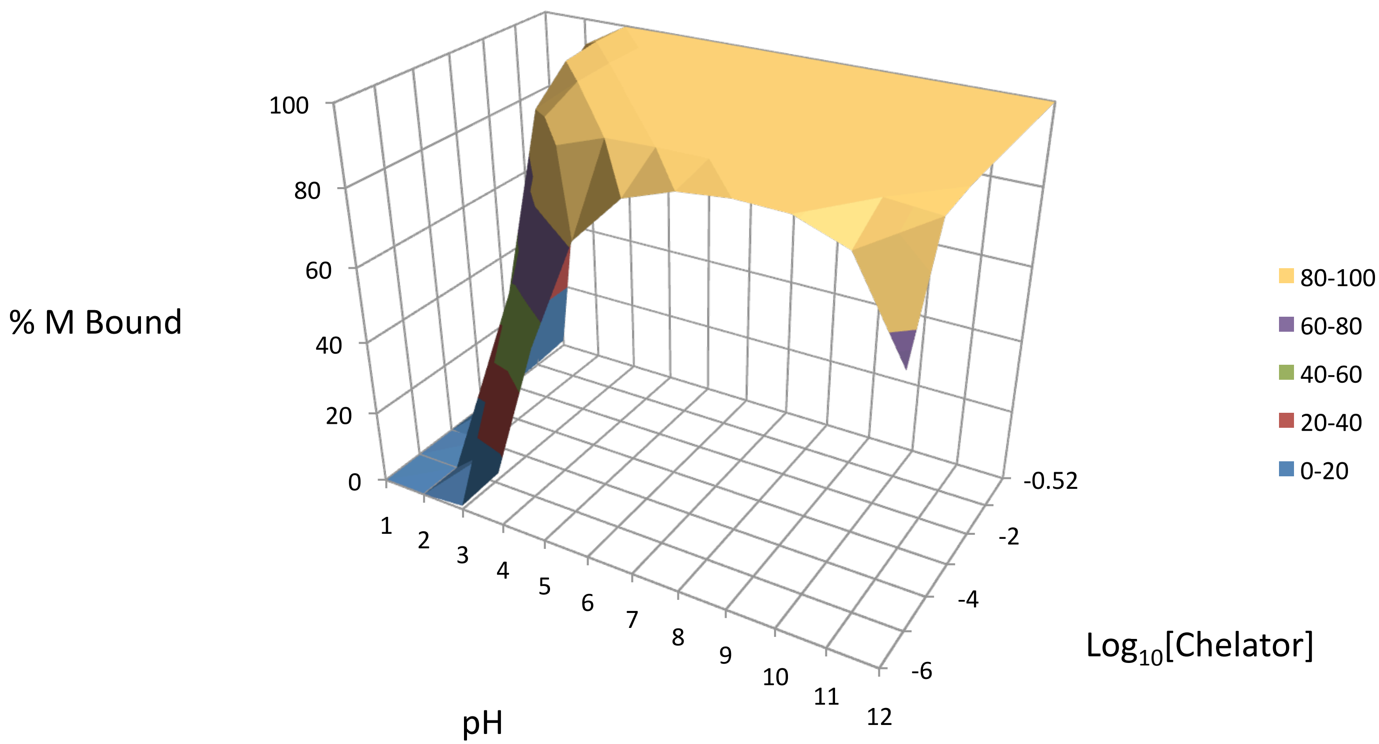


# Co – Citrate



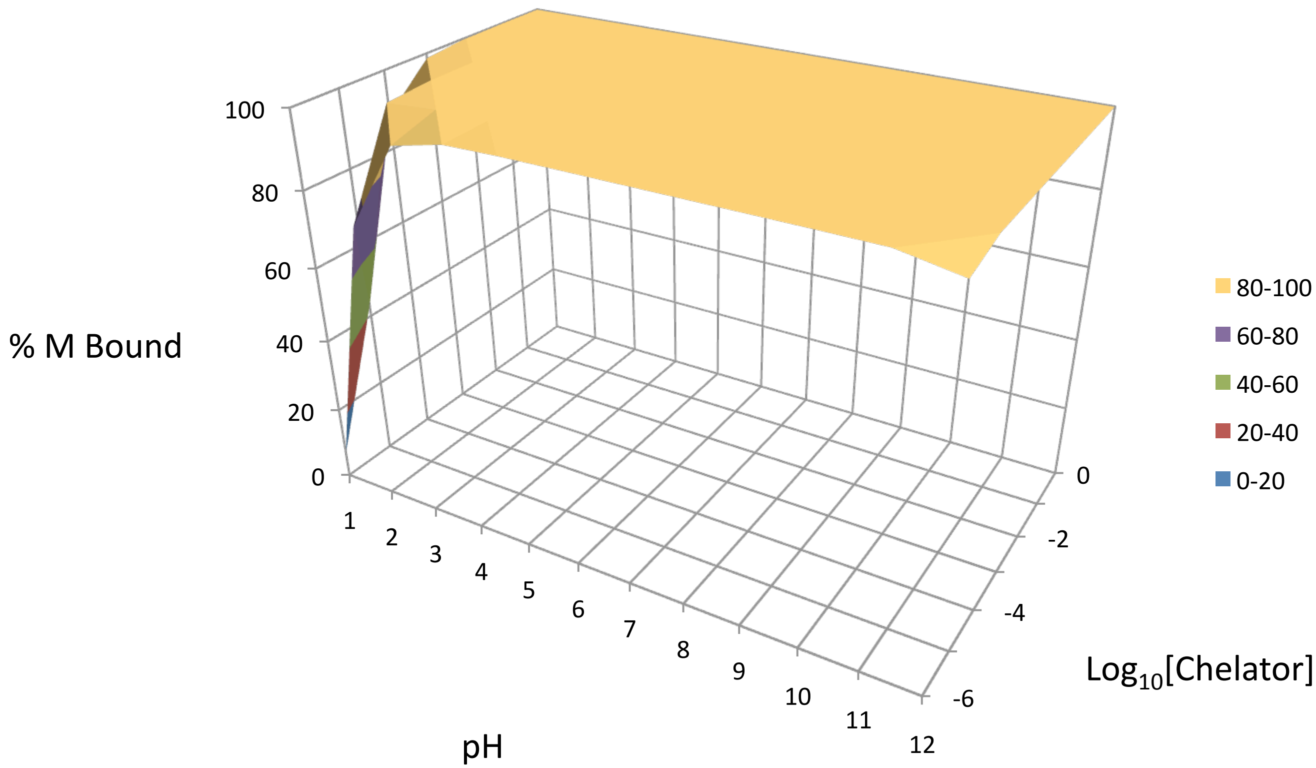
% M Bound
100
80
60
40
20
0
1
2
3
4
5
6
7
8
9
10
11
12
pH
-0.52
-1
-2
-3
-4
-5
-6
$Log_{10}$[Chelator]
80-100
60-80
40-60
20-40
0-20

# Co – NTA



% M Bound
100
80
60
40
20
0
1
2
3
4
5
6
7
8
9
10
11
12
pH
-0.52
-2
-4
-6
Log10[Chelator]
80-100
60-80
40-60
20-40
0-20

# Co – EDTA



% M Bound
100
80
60
40
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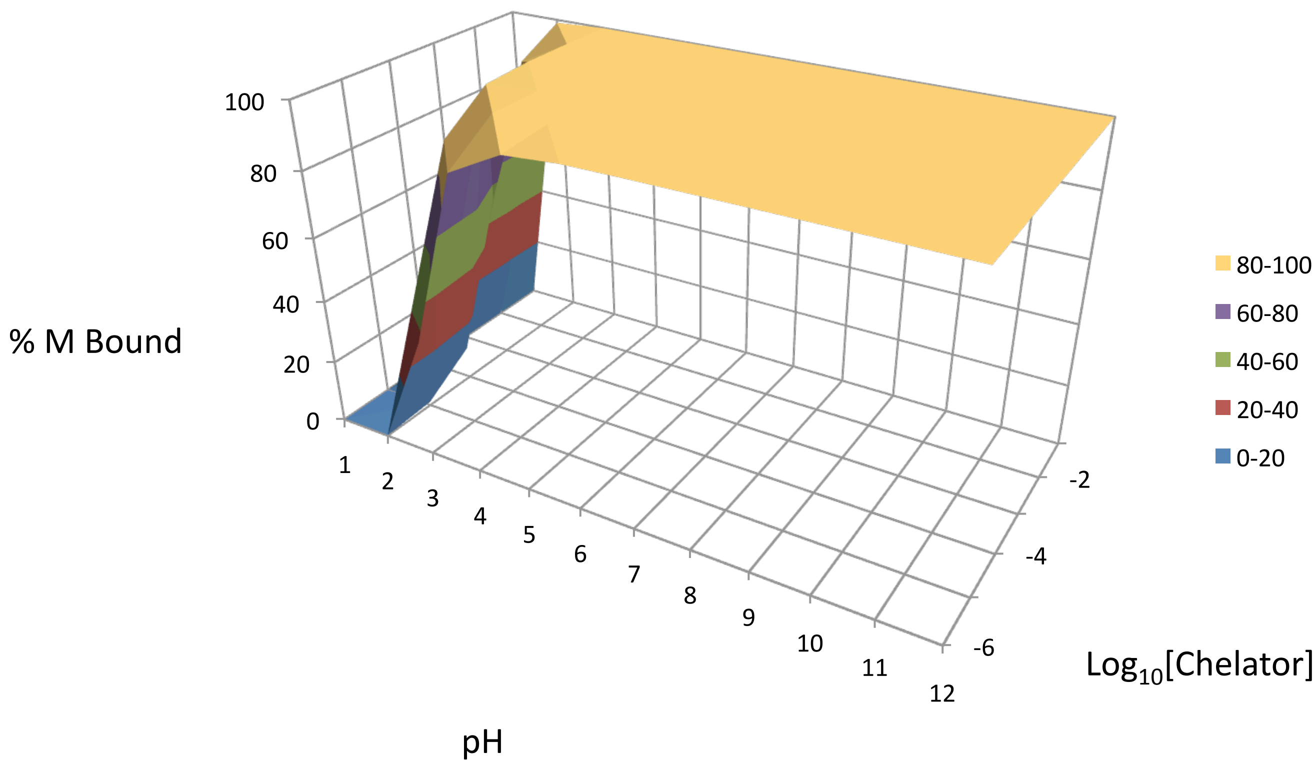
0
1
2
3
4
5
6
7
8
9
10
11
12
pH
0
-2
-4
-6
Log10[Chelator]
80-100
60-80
40-60
20-40
0-20

# Co – DTPA


% M Bound
100
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0
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2
3
4
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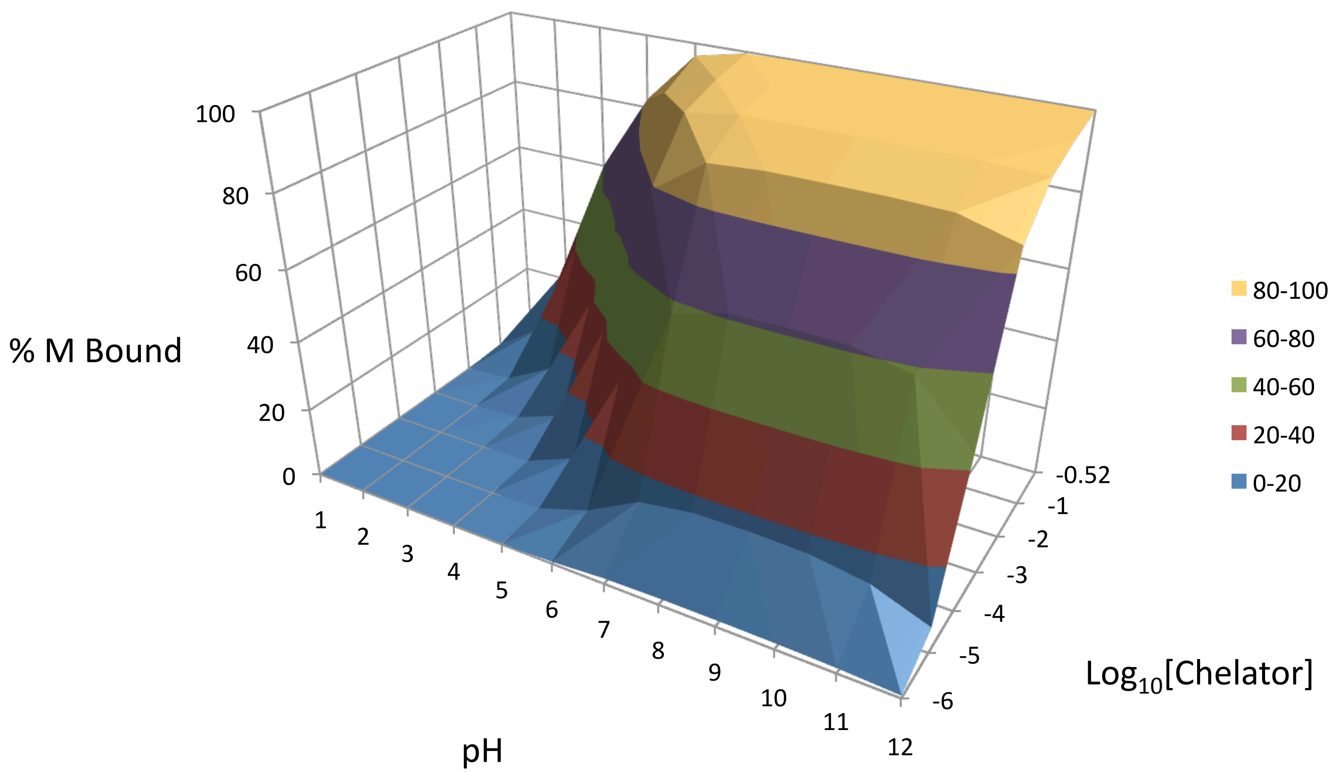
6
7
8
9
10
11
12
pH
-2
-4
-6
$Log_{10}$[Chelator]
80-100
60-80
40-60
20-40
0-20

# Sr – Citrate


% M Bound
100
80
60
40
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0
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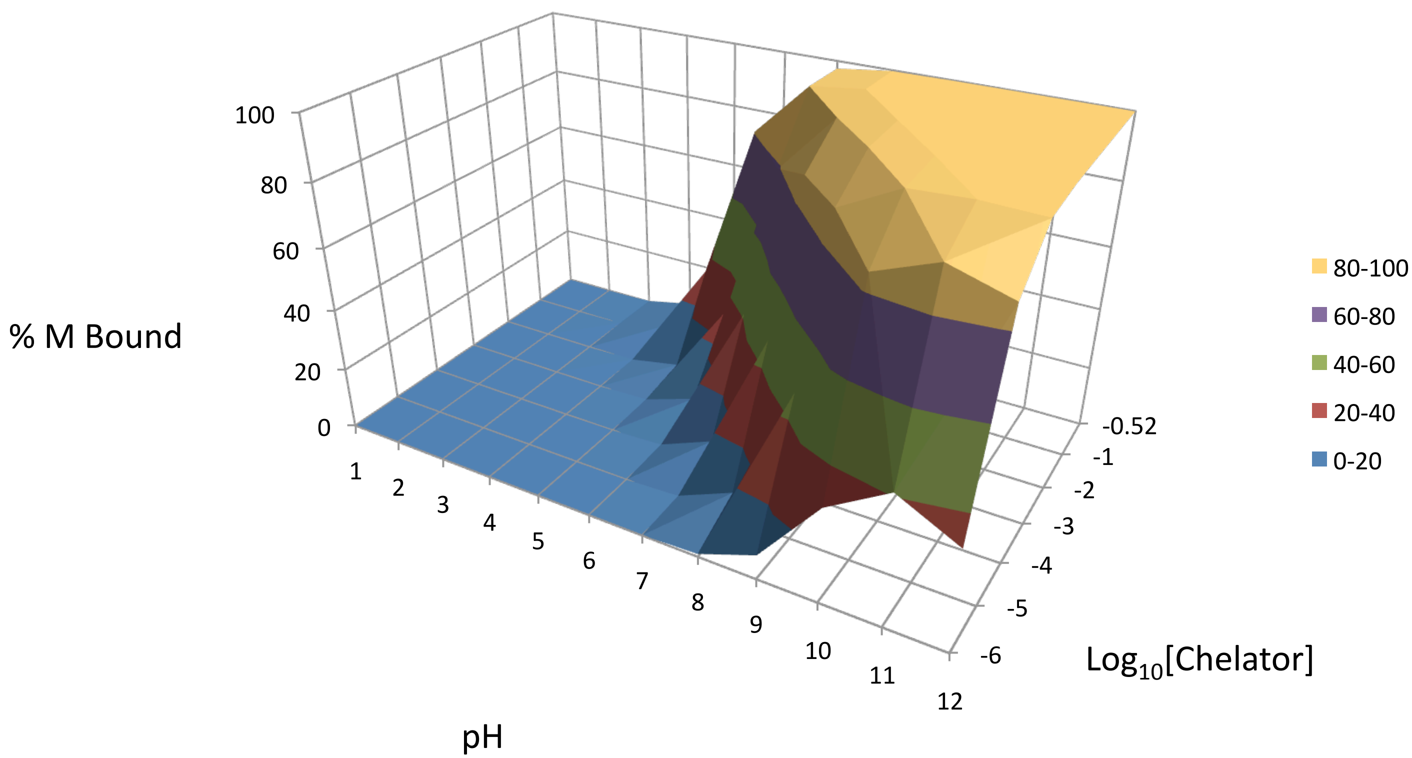
4
5
6
7
8
9
10
11
12
pH
-0.52
-1
-2
-3
-4
-5
-6
Log10[Chelator]
80-100
60-80
40-60
20-40
0-20

# Sr – NTA


% M Bound
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-3
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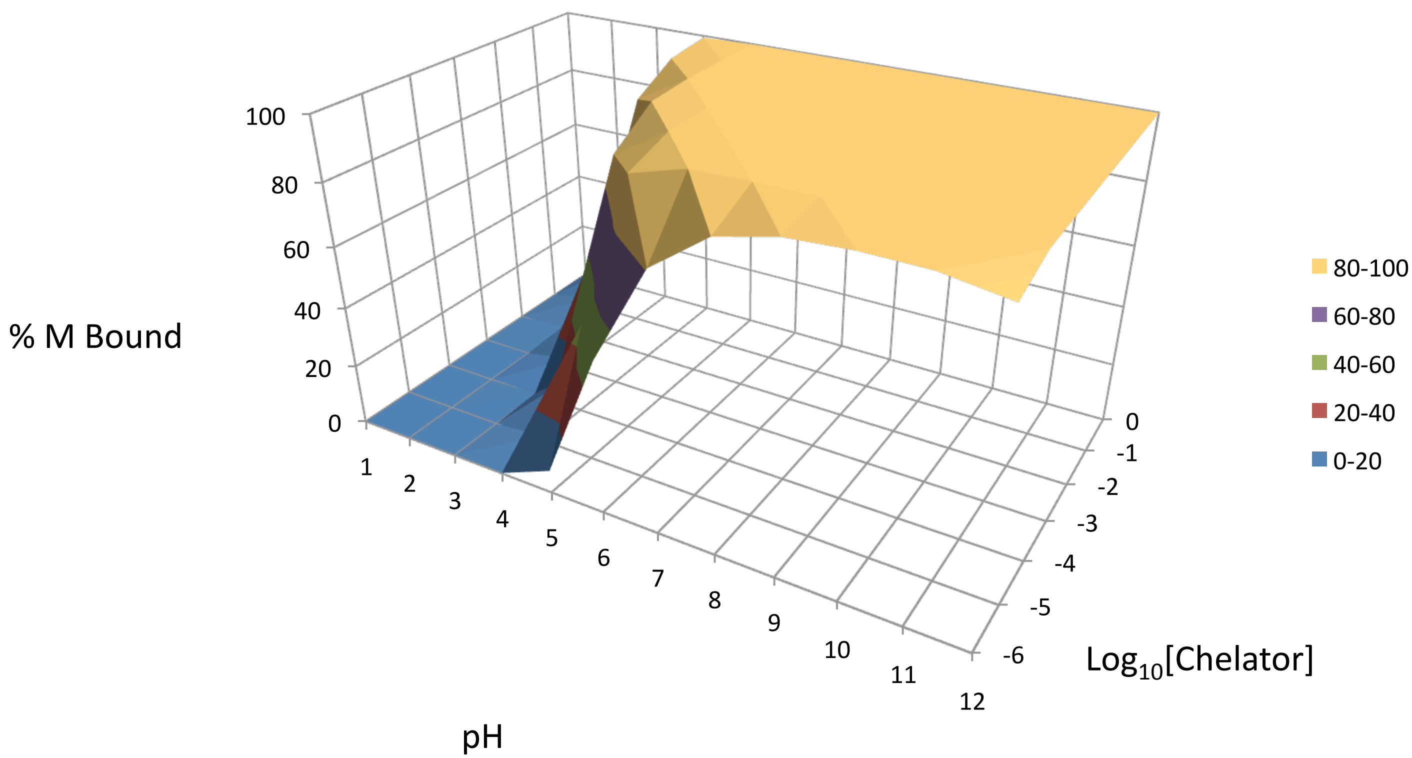
-5
-6
Log10[Chelator]
80-100
60-80
40-60
20-40
0-20

# Sr – EDTA



% M Bound
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11
12
pH
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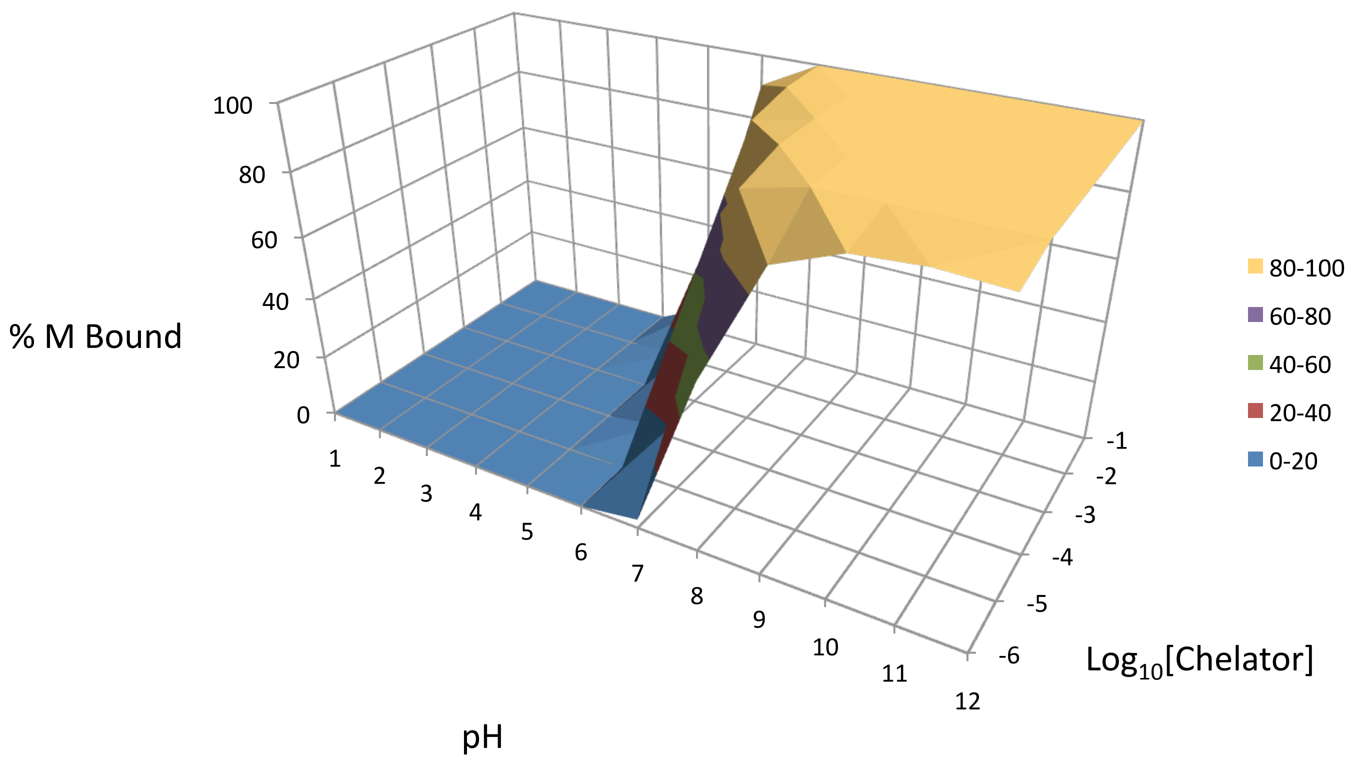
-1
-2
-3
-4
-5
-6
Log10[Chelator]
80-100
60-80
40-60
20-40
0-20

# Sr – DTPA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12
pH
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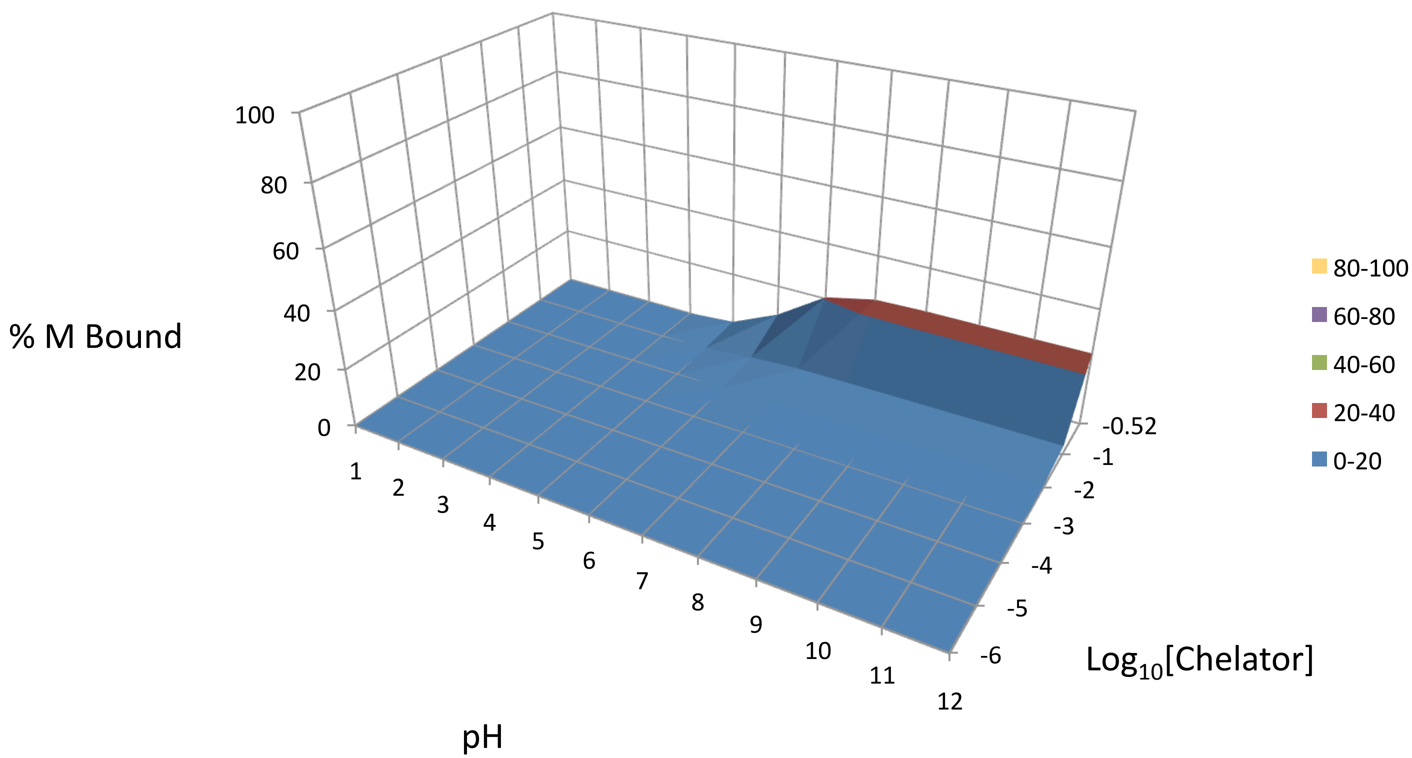
-2
-3
-4
-5
-6
Log10[Chelator]
80-100
60-80
40-60
20-40
0-20

# Cs – Citrate



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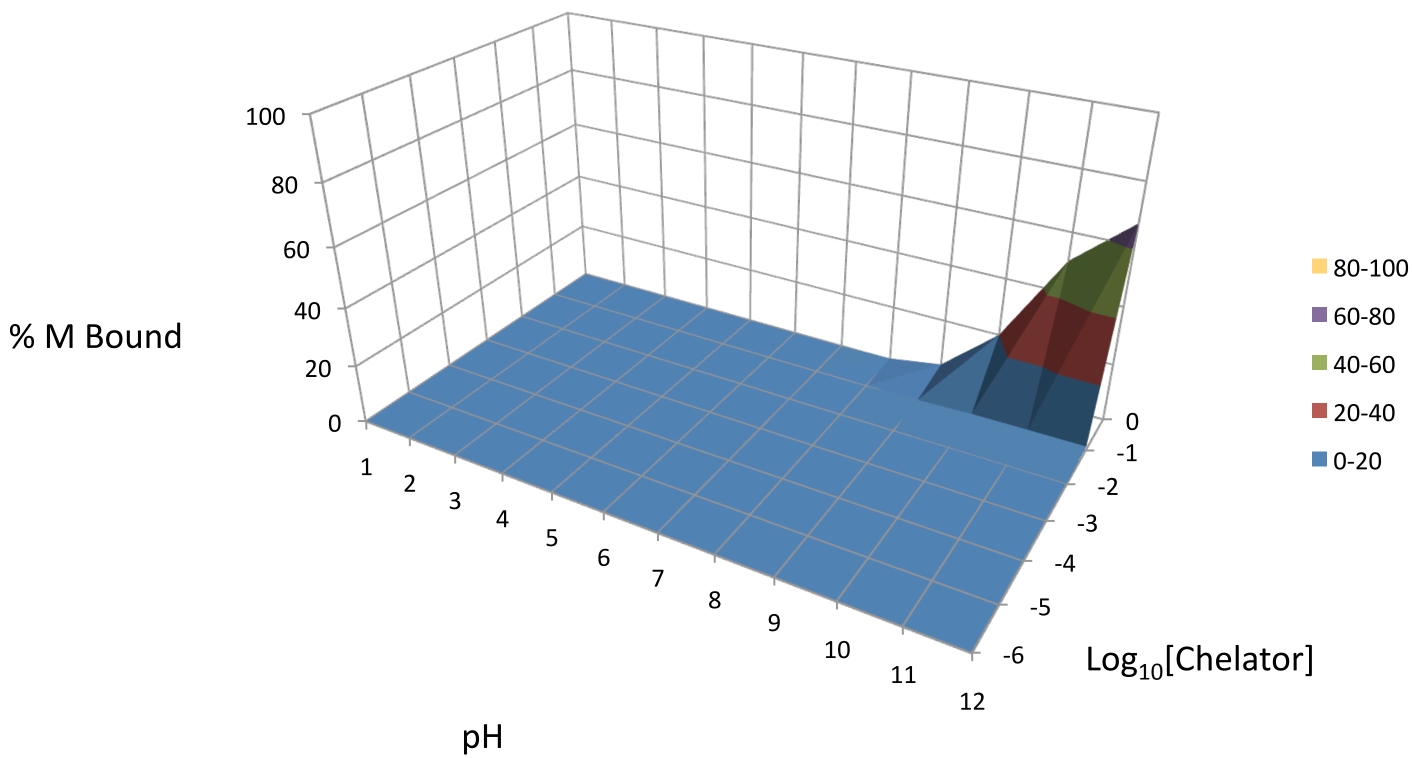
0-20

# Cs – EDTA



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## Disclaimer